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User's Guide to Diffusion/Kinetics (DIFKIN) Code

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USER'S GUIDE TO DIFFUSION/KINETICS (DIFKIN) CODE

Contract No. 68-02-0336

J. R. Martinez

October 1972

Prepared for
Environmental Protection Agency

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ABSTRACT

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1 INTRODUCTION

This manual contains instructions for using the computer code developed by General Research Corporation to model photochemical smog. The mathematical details of the code have been described in previous reports¹ and will not be repeated here. These instructions are thus limited to describing the features of the code which a user must know in order to successfully utilize the program. In addition, instructions are provided regarding certain modifications of the code.

DIFKIN is written in FORTRAN IV compatible with the IBM 360 system. The code is composed of a main program and twenty-five subprograms. Appendix A contains a list of the subprograms and a brief description of the function of each. The code operates in single-precision mode and requires approximately 16,000 words of core storage for execution.

Figure 1.1 is a diagram of the concepts used in the model. An air parcel moves along a path determined by the local prevailing wind speed

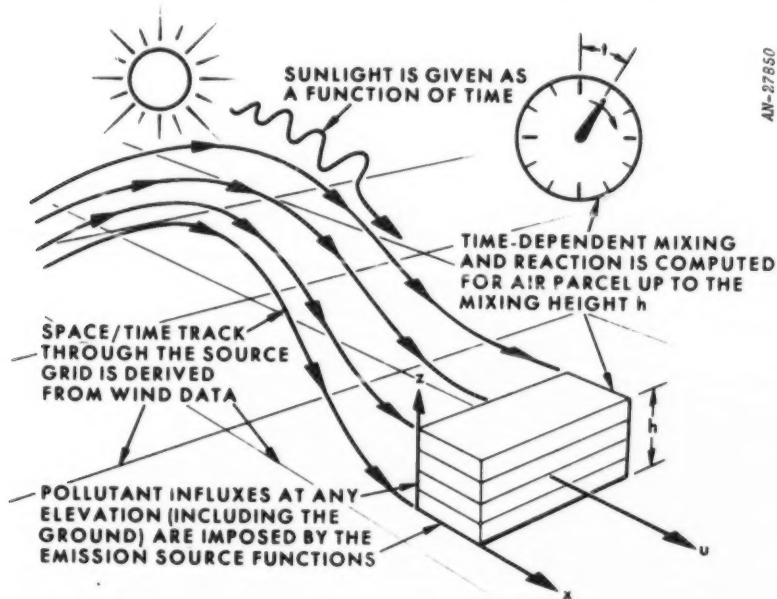
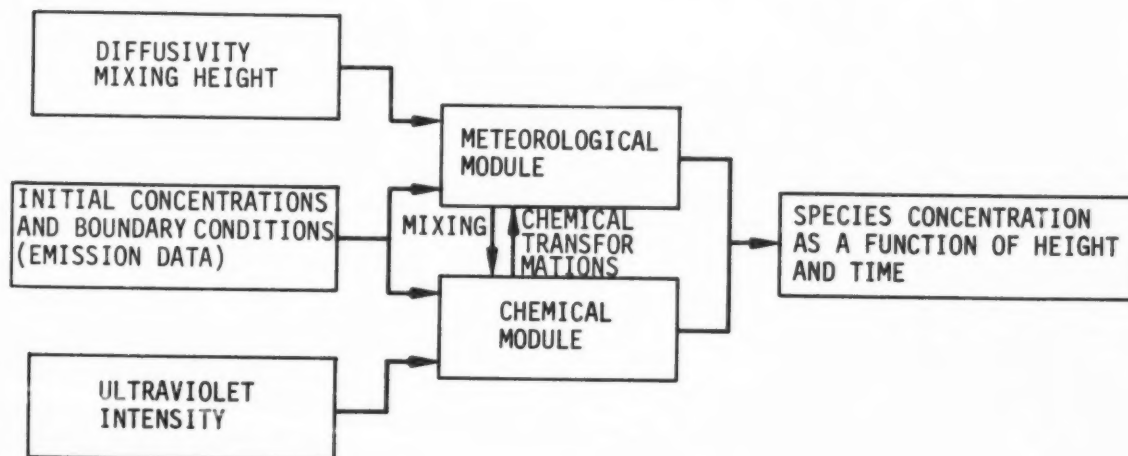


Figure 1.1. Schematic of Diffusion Model for Air Pollution Simulation

and direction at various times during the day. The air parcel is divided into a mesh of equally-spaced points in the vertical direction. As the air parcel moves over a region it receives pollutant emissions (fluxes) from the ground. The pollutants within the air parcel then undergo chemical reactions and mixing, with the incident sunlight driving several of the chemical reactions that occur. At each mesh point, the concentrations of several species of pollutants are computed; the output of the program consists of these concentrations as functions of time and height.

Figure 1.2 is a simplified flow chart showing DIFKIN input, processing, and output. The user provides meteorological and emission data, along with chemical rate constants and ultraviolet radiation intensity. The program computes the concentration of each of the species at each mesh point at specified time intervals along the path of the moving mass of air.



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Figure 1.2. Schematic Flow of DIFKIN Processing

It should be noted at this time that several subroutines used in the code are specialized for the chemical model and in general must be modified if the chemical model is changed. These subroutines are discussed in Sec. 4.1. However, changes in the numerical values of the chemical rate constants require no program modifications. Hence the rate constants can be changed at will simply by changing the appropriate input cards.

The meteorological inputs used in the program consist of inversion height data and the value of the diffusion coefficients. Wind speed and direction are not inputs to DIFKIN, but are used in an external auxiliary program which generates the proper emissions history for the specified wind trajectory. The auxiliary program produces as output a deck of fluxes along the trajectory, and these fluxes are the inputs to DIFKIN. A forthcoming version of DIFKIN will combine the current auxiliary programs with the version of DIFKIN described in this manual.

2 INPUTS

Before discussing the input parameters, we shall provide a description of the input process. This is necessary because the proper logical unit numbers must be assigned by the job control cards in order to run the program.

2.1 READING THE DATA CARDS

The process of reading the data cards is illustrated in Fig. 2.1. The data cards are read by subroutine PREDAT from the card reader, which PREDAT refers to as unit 3, e.g., READ (3,N) LIST. PREDAT reads the data until it detects an end-of-file mark, and then produces a listing of the data deck on the line printer, which is designated as unit 6, e.g., WRITE (6,N) LIST. Appendix B shows an example of the output produced by PREDAT. The subroutine also writes the data on a scratch peripheral memory unit such as a disk. This unit is designated by the logical unit number 5. After writing the data on unit 5, the subroutine rewinds unit

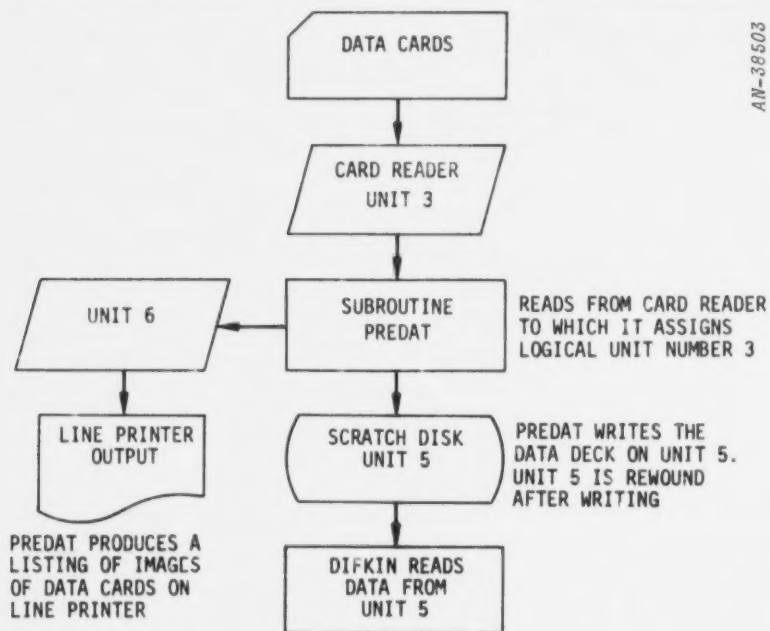


Figure 2.1. Process for Reading Data Used by DIFKIN

5 and the data are then ready to be read by DIFKIN, which reads from unit 5.

2.2 PROBLEM-CONTROL INPUTS

The input parameters of the program will be discussed in the order in which they are read by the code. The reader should refer to Appendix B, which contains a copy of the listing produced by PREDAT, in order to obtain a better picture of the actual structure of the data deck. Table 2.1 shows a list of the problem-control inputs along with a description of the function of each input variable, the name of the variable used in the code, and the format.

TABLE 2.1
PROBLEM-CONTROL INPUTS

Card Number	Variable Name Used in Code	Variable Function	Format	Remarks
1	TITLE	Label for each page of the output	(20A4)	May contain any comments user wishes to make. All 80 columns of the card may be used.
2	TIMIN	Initial time of run in minutes	(40X,F10.0)	
3	TSTOP	Final time of run in minutes	(40X,F10.0)	
4	DELT	Initial value of integration step size in minutes	(40X,F10.0)	The value of DELT is changed by the code during execution. The initial value should be small as a general rule, e.g., $\text{DELT} \leq 0.01$ minutes.
5	TSTMAX	Step size control parameter	(40X,F10.0)	See Sec. 6 for explanation of use.
6	TSTMIN	Step size control parameter	(40X,F10.0)	See Sec. 6 for explanation of use.
7	PRNTIN	Print interval	(40X,F10.0)	Concentrations are printed every PRNTIN minutes.
8	UPLIM	Upper limit on step size	(40X,F10.0)	The step size cannot be greater than UPLIM. A typical value is 0.5 min.
9	LOWLIM	Lower limit on step size	(40X,F10.0)	The step size cannot be smaller than LOWLIM. A typical value is 0.002 min.
10	DELZ	Height of one cell of space mesh in meters	(40X,F10.0)	$\text{DELZ} = H/(N-1)$ where H is the mixing depth and N is the number of vertical mesh points including the ground and the upper edge, where $N = \text{NOSTAT}$ (see card 25).
11	SUNTIM	Time interval in minutes for updating NO_2 photo-dissociation rate constant, k_1	(40X,F10.0)	The updating is done periodically since k_1 is a function of solar zenith angle. May have any dummy value if k_1 is held constant (see card 17). A typical value is 10 minutes.
12	FIXSTP	Integration step size fixed (YES) or variable (NO)	(40X,A4)	This is a Hollerith variable which is either YES or NO. In either case the word must start in column 41 and must contain no blanks.
13	KOUT	Print a list of all the time steps (YES) or not (NO)	(40X,A4)	See comment for card 12. The list contains the number of the time step, the time at which the integration step was performed, and the step size used. The list is written on logical unit 9, for output on the line printer via control cards after program execution is ended.

TABLE 2.1 (Cont.)

Card Number	Variable Name Used in Code	Variable Function	Format	Remarks
14	TIMOUT	Print at every print interval (see card 7) the number of integration steps carried out between print intervals, and the central processor time spent in the calculation (YES) or not (NO)	(40X,A4)	See comment for card 12. See Fig. 3.2b for an example of the output.
15	KEVERY	Print the concentrations for every integration step (YES) or not (NO)	(40X,A4)	See comment for card 12.
16	SPUNCH	Output concentrations on punched cards (YES) or not (NO)	(40X,A4)	See comment for card 12. The format used for punching is compatible with the format used by DIFKIN for reading initial concentrations.
17	QRATE	NO ₂ photodissociation rate constant variable (YES) or not (NO)	(40X,A4)	See comment for card 12. If QRATE = NO there is no updating of k_1 . See also comment for card 11.
18	IPLUX	Fluxes time-variable (YES) or constant (NO)	(40X,A4)	See comment for card 12.
19	QHTINV	Inversion height time-varying (YES) or constant (NO)	(40X,A4)	See comment for card 12. See Sec. 2.3.7 for explanation.
20	NUMSTP	Maximum number of integration steps	(40X,I10)	Integer variable. Program execution is terminated if NUMSTP is exceeded. A message is printed to this effect to advise user.
21	NOREAC	Number of chemical reactions	(40X,I10)	Integer variable. Cannot exceed 20 with present array dimensions.
22	NOSP1	Total number of species, including reactive and non-reactive species	(40X,I10)	Integer variable. Cannot exceed 20 with present array dimensions.
23	NSTDY	Number of reactive species in steady state which are to be explicitly calculated	(40X,I10)	Integer variable.
24	NTRACE	Number of non-reactive (tracer) species	(40X,I10)	Integer variable. This number is either zero or one. A zero means no tracer species is input.
25	NOSTAT	Number of vertical mesh points to be used	(40X,I10)	Integer variable. Cannot exceed 10 with present array dimensions.

2.3 ADDITIONAL INPUTS

The remaining inputs required by the program are discussed below. All the inputs are presented in Table 2.2, following the same format as Table 2.1 except that the card number is now changed to a group number. This is because the number of cards in these inputs varies, depending on the number of species and the number of mesh points. Each of the nine groups of inputs is discussed in the following sections.

2.3.1 Species Name and Molecular Weight

After card number 25, the name and molecular weight of each species are input. These are input on the same card using format (40X, A4, 6X, F10.2). The name and molecular weight are stored in arrays SPEC and WTMOLE, respectively. The number of cards input is NOSPl (see Table 2.1, card 22).

The order in which the species are input is important for program execution. The program must have

- All active species first (in any order)
- NSTDY steady-state species next (in any order)
- The tracer species last (if any declared by NTRACE, card 20)

The so-called active species are those whose concentrations are computed by integration of the rate equations. This is in contrast to the steady-state species, which are obtained algebraically.

This input step determines the order of appearance of all the species in any subsequent inputs which are tied to the species.

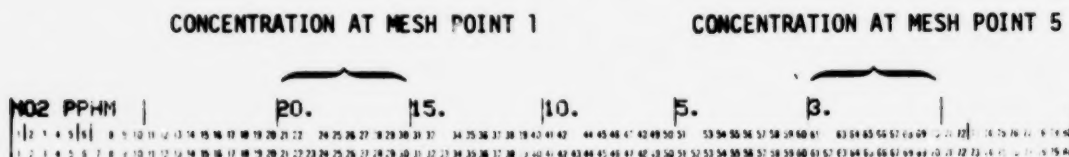
2.3.2 Initial Concentrations for Each Species

The initial concentration of each species at each mesh point in parts per hundred million (pphm) is input next. This is stored in array PPHM, and PPHM(i,j) denotes the concentration of the jth species at the i-th mesh point. The format used is (20X, 5E10.4) and the input for each

TABLE 2.2
ADDITIONAL INPUTS

Group Number	Variable Name Used in Code	Variable Function	Format	Remarks
26	SPEC, WTMOLE	Species name and molecular weight	(40X,A4.6X,F10.2)	Each card contains the name and molecular weight of one species. Thus the number of cards required is NOSPL (see card 22). See Sec. 2.3.1.
27	PPHM	Initial concentration of each species at each mesh point in pphm	(20X,5E10.4)	See Sec. 2.3.2.
28	RATKON	Rate constants for chemical reactions in units consistent with species concentration, e.g., $\text{pphm}^{-1}\text{min}^{-1}$	(40X,F10.0)	One card per reaction makes a total of NOREAC cards in this group. See Sec. 2.3.3.
29	REACT	Description of chemical reactions in the model.	(8A4)	See Sec. 2.3.4.
30	STOYKR, STOYKP	Stoichiometric coefficients for reactants and products	(2F10.0)	See Sec. 2.3.5.
31	RATK1	Table of rate constants of NO_2 photodissociation reaction, k_1 , in minute^{-1}	(20X,E15.5)	See Sec. 2.3.6. Required only if QRATE = YES (card 17).
32	HTINV	Table of diffusion coefficients as functions of time and altitude, in meters squared per minute	(20X,5E10.4)	See Sec. 2.3.7. Required only if QHTINV = YES (card 19).
33	FLXTIM	Table of times when fluxes are updated, in minutes	(40X,F10.0)	See Sec. 2.3.8. Required only if IFLUX = YES (card 18).
34	FLXWAL, VALWAL, FLXDGE	Boundary conditions for each species: flux at ground, concentration at ground, and flux at upper edge, respectively.	(30X,3E15.5)	See Sec. 2.3.9.

species is the concentration at each mesh point from bottom to top, with up to five mesh points to a card as indicated by the diagram below.



The number of cards per species is equal to $[(\text{NOSTAT} - 1)/5] + 1$, where NOSTAT is the number of space mesh points (see Table 2.1, card 25), and the notation $[\cdot]$ denotes the integral part of the expression within the brackets. Cards for the tracer species must not be included if NTRACE = 0 (card 24).

The initial concentrations of the steady-state species need not be input because the code automatically computes them. However, the user must include cards in the input deck for each steady-state species. In our sample run, four species are designated as being in steady-state: NO_3 , N_2O_5 , OH, and RO_2 . Referring to Appendix B, cards 40-43 show that the initial concentrations of these species have not been specified. The initial concentrations of these species will be computed by the code from the given initial concentrations of the five active species, NO, HC, NO_2 , O_3 , and HNO_2 . Figure 3.2a in Sec. 3.2 shows the computed initial concentrations of the steady-state species.

2.3.3 Rate Constants for Chemical Reactions

These are input one to a card, i.e., one card per reaction, using format (40X, F10.0). They are stored in array RATKON. There is a total of NOREAC rate-constant data cards. The NO_2 photodissociation reaction is the first one in the kinetic model as currently structured. However, it may be assigned any position provided that any subsequent inputs are consistent with the assigned order.

2.3.4 Description of Chemical Reactions in the Model

This input is for information only and plays no role in the computation. The input is in Hollerith form using format (8A4), one reaction to a card. The user may make any notations in the allotted space, the first 32 columns of the card. Appendix B, cards 60 to 75, shows an example of these data cards. There is a total of NOREAC cards and the symbols are stored in array REACT. This input need not be repeated when multiple runs are made (see Sec. 4.2 for multiple-run procedures).

2.3.5 Specification of the Chemical System (Stoichiometric Coefficients)

A set of chemical reactions is specified by a set of NOREAC stoichiometric equations of the form:

$$\sum_{j=1}^s v_{ij} M_j \xrightarrow{k_i} \sum_{j=1}^s v'_{ij} M_j, \quad i = 1, 2, \dots, \text{NOREAC}$$

where

M_j = chemical formula of j th species

v_{ij} = stoichiometric coefficient of reactant species

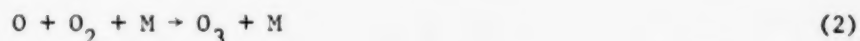
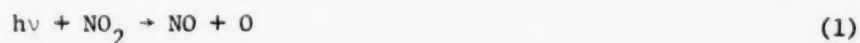
v'_{ij} = stoichiometric coefficient of product species

k_i = rate constant of i th reaction [RATKON(i), see Sec. 2.3.3]

s = number of chemically active species, i.e.,

$s = \text{NOSP1} - \text{NTRACE}$

The input of the DIFKIN code consists of the stoichiometric coefficients v_{ij} and v'_{ij} . These coefficients are input two per card, v_{ij} and v'_{ij} , using format (2F10.0). The ordering scheme is best explained by an example. Consider the reaction set:



The stoichiometry input would be as follows:

Card Number	Species	Reaction Number	Input Using Format (2F10.0)	
			ν	ν'
1	NO ₂	1	1.	0
2		2	0	0
3		3	0	1.
4	NO	1	0	1.
5		2	0	0
6		3	1.	0
7	O ₃	1	0	0
8		2	0	1.
9		3	1.	0

And so on for the other species. Thus it should be clear that the stoichiometric coefficients are grouped by species and that for each species the stoichiometry must be specified for all reactions. Hence, for NOREAC reactions and (NOSP1 - NTRACE) species we have (NOREAC) × (NOSP1 - NTRACE) cards in the stoichiometric matrix input. We note that the order of the species-reaction groups in this input must be consistent with the name ordering, the concentration ordering, and so forth. Also, it can be seen that this kind of input is very general and affords great flexibility in specifying various chemical systems. The stoichiometric matrix is input only once when making multiple runs (see Sec. 4.2 for an explanation of multiple-run procedures).

2.3.6 Input for Variable NO₂ Photodissociation Rate Constant

These data are read only if QRATE = YES (see Table 2.1, card 17); otherwise they must not be included in the deck.

The format used for these cards is (20X, E15.5) and the rate constants are input one to a card, one card for each time. They are stored in array RATK1 and the maximum number of cards is 100. The time interval between updates is that specified on card 11 of Table 2.1. The last card of the table must contain a negative number to stop the code from reading.

If QRATE = YES, then the first card on the input table must contain the value of the rate constant which corresponds to the initial time of the run. The program updates RATKON(1) (see Sec. 2.3.3) automatically to reflect this fact. Hence, the value of the rate constant input in Sec. 2.3.3 need not be the correct value inasmuch as it will be updated when RATK1 is read. The updating is done by a call to the subroutine UPRATE.

2.3.7 Table of Diffusion Coefficients as Functions of Time and Altitude

These data are read only if QHTINV = YES (see Table 2.1, card 19); otherwise they must not be included in the deck.

The format used for these cards is (20X, 5E10.4). Each card contains up to five numbers arranged in columns 21-30, 31-40, 41-50, 51-60, 61-70. The diffusivities are updated as functions of time and each entry of the input table must contain the following: the update time, the inversion height, and the diffusivities at the various points in the mesh. (The inversion height is informational only and is not used in the computation, so it really need not be input. It has been included for the sake of completeness.) The number of diffusivities is equal to NOSTAT + 1 since each diffusivity must be specified at the midpoint of each cell as well as at the ground and at the upper edge of the space mesh. The table is arranged as follows:

Card 1--Columns 21-30	Update time in minutes from start of run
Columns 31-40	Inversion height in meters
Columns 41-50, 51-60, 61-70	Diffusivity at ground and at the next two points in the mesh, in meters squared per minute
Card 2--Columns 21-30, etc., and thereafter	Diffusivities at other points in the mesh, 5 to a card

Thus, for each update time there must be a set of diffusivities. If the number of mesh points is 5, for example, two cards per update time will be needed. The last group of cards in the array must contain a negative number in the position allocated for the time in order to stop the code from reading.* The maximum number of update times allowed is 20 and the table is stored in array HTINV.

2.3.8 Table of Flux Update Times

This table contains the times when the fluxes are to be updated, in minutes from the start of the run. The first entry of the table must match the initial time of the run, TIMIN (Table 2.1, card 2). The last entry of the table must be equal to or greater than TSTOP (Table 2.1, card 3). The times are stored in array FLXTIM, and the format used is (40X,F10.0). The very last card of this group must contain a negative number in Columns 41-50 to stop the code from reading. The maximum number of cards allowed is 100, under present dimensions.

2.3.9 Boundary Conditions

Two kinds of boundary conditions are allowed in the code, a flux boundary condition and a wall boundary condition. In the former, fluxes

* Note that this last group must have the same number of cards as the preceding ones, even though only the first carries any information.

are specified at the ground and at the upper edge of the mesh. In the latter, a particular value of concentration is specified at the ground. For reactive species, only the flux condition is allowed. For the tracer species, the user may specify either of the two kinds of boundary conditions.

These inputs are stored in arrays FLXWAL, FLXDGE, and VALWAL, where the first one denotes the flux at the ground, the second the flux at the upper edge of the air parcel, and the third the concentration at the ground. Normally, FLXDGE is set to zero since no mass is allowed to flow through the upper boundary of the air parcel; this is equivalent to saying that the pollutants are trapped below the inversion base.

The boundary conditions are read as needed when the updating time has arrived. Hence, there is no need to provide storage space for the boundary conditions at various times. The order in which the boundary conditions are input must be consistent with the order of the update times previously read in (see Sec. 2.3.8). The boundary conditions are read and updated by subroutine UPFLUX, the main program being designed to call UPFLUX at the appropriate time. For each time, one card specifies the boundary conditions for one species in the format (30X, 3E15.5). The order of the boundary conditions on each card is FLXWAL, VALWAL, FLXDGE in Columns 31-45, 46-60, 61-75, respectively. The units of the flux depend on the units used for the species concentration. In our case the program performs the computations in mass-fraction units, and the fluxes are thus specified as volumetric fluxes with units of meters/minute. Any scaling that needs to be done on the boundary conditions must be done by UPFLUX since there is no provision for scaling in the main program. In our case the fluxes are scaled by a factor of 10^8 in order to preserve accuracy in the computation.

For the tracer species, the value of VALWAL is significant if it is other than zero. A zero value of VALWAL indicates to DIFKIN that no wall boundary condition is being used (see subroutine CRANK).

Appendix B, lines 339 to 416, shows a typical set of inputs for flux boundary conditions. In this case only NO and HC have fluxes at the ground and no flux penetrates the upper edge of the air parcel. Note that the fluxes on lines 339 and 340 appear also in Fig. 3.1d, scaled by a factor of 10^8 . The program "knows" that only two fluxes need to be read because subroutine UPFLUX, which reads the fluxes, is written to read only two fluxes. If more or fewer fluxes are input, UPFLUX must be modified to reflect this fact.

3 OUTPUTS

DIFKIN produces two kinds of output: line printer and punched card. The latter is optional, being produced at the command of the user (Table 2.1, Card 16). The printed output is shown in the accompanying figures. The interpretation of the output is discussed below.

The main line printer output consists of the following:

1. Images of the data cards in the input deck (Appendix B)
2. Summary of input data (Figs. 3.1a through 3.1e)
3. Concentrations of the various species as a function of time and height (Figs. 3.2a and 3.2b).

In addition to these three items, several utility outputs are available for the convenience of the user. These are described in Sec. 3.3.

The punched-card output consists of the species concentrations as functions of time and height. The punched cards are generated at the same time the species concentrations are printed. The format of the cards matches the format used for input, group 27 of Table 2.2.

3.1 SUMMARY OF INPUT DATA

The line printer output shown in Fig. 3.1 consists of a summary of the input data used in the problem. At the top of the first page, Fig. 3.1a, the run label appears first. This appears on every page of the output and corresponds to the data on the first card of the input deck. Also appearing on the first line are the central processor time (CP TIME) in seconds, the date of the run, and the page number. Proceeding down the page, several input quantities are listed, beginning with the initial time and ending with the lower limit fractional change used to control the step size. On Fig. 3.1a these entries are cross-referenced to Table 2.1.

The next listing of inputs consists of the reactant and product stoichiometric matrices, together with the rate constant of each reaction.

The stoichiometric matrix listings shown in Figs. 3.1a and 3.1b are interpreted as follows. The reactions correspond to the rows of the matrix and the species to the columns. Thus consider reaction 2: the stoichiometric matrix of reactants, Fig. 3.1a, says that only species NO and OZON appear in reaction 2, each with unit stoichiometric coefficient. The rate constant of reaction 2 is given as $.267 \text{ pphm}^{-1} \text{ min}^{-1}$. The stoichiometric matrix of products, Fig. 3.1b, is read in the same way as the matrix for reactants. Thus for reaction 2 the product is one molecule of NO₂. The schematic reaction obtained from reading the stoichiometric matrices is (1)NO + (1)OZON → (1)NO₂, where the quantities in parentheses are the stoichiometric coefficients. (Note that this schematic reaction does not balance. The true reaction is $\text{NO} + \text{O}_3 \rightarrow \text{NO}_2 + \text{O}_2$, but O₂ is not carried explicitly in the computation, hence the omission.)

Figure 3.1c shows a list of all the reactions used in this sample run. These reactions correspond to the schematic reactions defined by the stoichiometric matrices, of course. Thus the listing in Fig. 3.1c can be used to interpret the stoichiometric matrices and vice versa.

Figure 3.1d lists the species in the prescribed order, together with the boundary conditions at the initial time and the molecular weight of each species. In the example shown, only NO and HC (hydrocarbon) have fluxes at the ground (FLXWAL) and no flux is permitted to cross the upper edge of the air parcel (FLXDGE = 0). (See Sec. 2.3.9 for information regarding VALWAL.) Note that the value of FLXWAL shown for NO and HC is equal to that shown on cards 339 and 340 of Appendix B scaled by a factor of 10^8 .

The last listing of inputs, shown in Fig. 3.1e, is a list of the initial values of the diffusivities. These values correspond to the quantities shown in cards 285 and 286 of Appendix B.

DIFIN SAMPLE RUN =

CP TIME = 17.1R DATE 02/25/73 Page 1

INPUT DATA FOR VERTICAL DIFFUSION PROBLEM WITH PHOTOCHEMISTRY

INITIAL TIME IS 0. MINUTES (INPUT CARD 2)
 FINAL TIME IS 3.00000E+02 MINUTES (INPUT CARD 3)
 TIME STEP SIZE IS 1.00000E+02 MINUTES (INPUT CARD 4)
 VERTICAL MESH INCREMENT IS 1.15000E+02 METERS (INPUT CARD 10)
 NUMBER OF REACTIONS IS 16 (INPUT CARD 21)
 NUMBER OF SPECIES IS 9 (INPUT CARD 22)
 NUMBER OF SPECIES IN STEADY STATE IS 4 (INPUT CARD 23)
 NUMBER OF TRACER SPECIES IS 0 (CANNOT EXCEED 1) (INPUT CARD 24)
 NUMBER OF VERTICAL MESH POINTS IS 4 INCLUDING THE GROUND AND THE EDGE (INPUT CARD 25)

STEP SIZE CONTROLS

UPPER LIMIT FRACTIONAL CHANGE IS 3.00000E-02 (INPUT CARD 5)
 LOWER LIMIT FRACTIONAL CHANGE IS 1.00000E-02 (INPUT CARD 6)

REACTION	NO NO2	HC	NO2	O2ON	HN02	NO3	N2O5	OH	RATE COEFFICIENT
									(DDM/UNIT)
1	0.0 0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	5.42370E-01
2	1.0 0.0	0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.24700
3	0.0 0.0	1.0	0.0	0.0	0.0	0.0	0.0	0.0	1.00000E-01
4	0.0 0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.0	5.0.000
5	1.0 1.0	0.0	0.0	0.0	0.0	0.0	0.0	0.0	1000.000
6	0.0 1.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	2.0000
7	1.0 0.0	0.0	0.0	0.0	0.0	0.0	0.0	1.0	15.000
8	0.0 0.0	0.0	1.0	0.0	0.0	0.0	0.0	1.0	30.000
9	0.0 0.0	1.0	0.0	1.0	0.0	0.0	0.0	0.0	4.00000E-01
10	0.0 0.0	0.0	0.0	0.0	1.0	0.0	0.0	0.0	2.00000E-01
11	0.0 0.0	0.0	1.0	1.0	0.0	0.0	0.0	0.0	5.00000E-01
12	0.0 0.0	0.0	1.0	0.0	0.0	1.0	0.0	0.0	45.000
13	0.0 0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	14.000
14	0.0 0.0	0.0	0.0	0.0	0.0	0.0	1.0	0.0	40.500
15	1.0 0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.00000E-01
16	0.0 0.0	0.0	1.0	0.0	0.0	0.0	0.0	0.0	1.00000E-01

Figure 3.1a. Summary of Input Data

REACTION		-- PRODUCT STOICHIOMETRY --						
1	1.00 0.00	0.00	0.00	1.00	0.00	0.00	0.00	0.00
2	0.00 0.00	0.00	1.00	0.00	0.00	0.00	0.00	0.00
3	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
4	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
5	0.00 0.00	0.00	1.00	0.00	0.00	0.00	0.00	.13
6	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
7	0.00 0.00	0.00	0.00	0.00	1.00	0.00	0.00	0.00
8	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
9	0.00 1.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
10	1.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	1.00
11	0.00 0.00	0.00	0.00	0.00	0.00	1.00	0.00	0.00
12	0.00 0.00	0.00	0.00	0.00	0.00	0.00	1.00	0.00
13	0.00 0.00	0.00	1.00	0.00	0.00	1.00	0.00	0.00
14	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00
15	0.00 0.00	0.00	0.00	0.00	2.00	0.00	0.00	0.00
16	0.00 0.00	0.00	0.00	0.00	0.00	0.00	0.00	0.00

AM-28504 Cont.

Figure 3.1b. Summary of Input Data: Stoichiometric Matrix of Product Species

REACTIONS

1. PHOTON + NO2 = NO + O3
2. NO + O3 = NO2 + O2
3. O + HC = BRN2
4. OH + HC = BRN2
5. RO2 + NO = NO2 + .129*OH
6. RO2 + NO2 = PAN
7. OH + NO = HNO2
8. OH + NO2 = HNO3
9. O3 + HC = RO2
10. PHOTON + HONO = OH + NO
11. NO2 + O3 = NO3 + O2
12. NO3 + NO2 = N2O5
13. N2O5 = NO3 + NO2
14. N2O5 + H2O = 2HNO3
15. NO + NO2 + H2O = 2HNO2
16. NO2 + PARTICLES = PRODUCTS

Figure 3.1c. Summary of Input Data: Description of Chemical Reactions Used in Model

SPECIES	FIXVAL	VALVAL	FLXINDE	MOLE WT
NO	3.07086E+01	0.	0.	3.00100E+01
HC	9.44323E+01	0.	0.	7.22000E+01
NO2	0.	0.	0.	4.60100E+01
O3	0.	0.	0.	4.80000E+01
HNO2	0.	0.	0.	4.70000E+01
NO3	0.	0.	0.	6.20000E+01
N2O5	0.	0.	0.	1.00000E+02
OH	0.	0.	0.	1.70000E+01
RO2	0.	0.	0.	4.61000E+01

Figure 3.1d. Summary of Input Data: Boundary Conditions and Molecular Weights

DIFRIN SAMPLE RUN =

CP TIME = 17.61 DATE 02/25/79 PAGE 4

INITIAL DIFFUSION COEFFICIENTS

VALUES SHOWN ARE FOR POINTS HALFWAY BETWEEN STATIONS

STATION	HEIGHT (METERS)	DIFFUSIVITY
1	0.00	30.000000
		30.000000
2	114.00	30.000000
		30.000000
3	238.00	30.000000
		30.000000
4	362.00	30.000000
		30.000000
5	486.00	30.000000

AB-18204 CONCL.

Figure 3.1e. Summary of Input Data: Initial Diffusivity Profile

3.2 OUTPUT OF SPECIES CONCENTRATIONS

Figures 3.2a and 3.2b show the output of the species concentrations produced by DIFKIN. Figure 3.2a contains the initial concentrations which have been input by the user. These correspond to cards 35-39 of Appendix B. Each column of the output corresponds to one species, and each row corresponds to a given height. The first row shows a height of zero meters and is, of course, the ground. Subsequent rows correspond to increasing altitudes. Note that the first column contains two species, NO and RO2; these are read in the order indicated by the order of the name of the species, i.e., first NO and then RO2. The species are printed folded together in multiples of 8. Hence, for 17 species the first column would contain 3 species, and so on.

Figure 3.2b shows the output of the computation after 30 minutes of real time have elapsed. Because the print interval, PRNTIN (card 7 in Table 2.1 and Appendix B), is equal to 30 minutes the program will print the species concentrations and the time every 30 minutes. Some additional information is printed on the page: the value of the diffusion coefficient at the ground, the value of k_1 , and the fluxes of NO, HC, and CO, the last being the tracer species. Since we have no tracer species in this example, the CO flux is set to zero. Note that the value of k_1 shown in Fig. 3.2b matches the quantity shown on card 220 of Appendix B. Similarly, the fluxes correspond to those shown on lines 349 and 350 of Appendix B scaled by 10^8 . Clearly, the value of k_1 and the flux are not the values of those quantities at 0700, which corresponds to 30 minutes. This is simply because the printing is done before updating k_1 and the fluxes. After printing, the program will update these quantities and proceed to the next integration step.

The last line of Fig. 3.2b shows that it took 121 integration steps to get from 0 to 30 minutes of real time (cycle No. 1), and that this took 19.439 seconds of central processor time. This output is optional and is controlled by TIMOUT (Table 2.1, Card 14).

DIFKIN RAIBLE RUN -

CP TIME = 17.65 DATE 02/25/73 PAGE 4

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INITIAL PROFILES OF CONCENTRATIONS-PPHM

HEIGHT-M.	NO	NO2	HC	NO2	OZON	HNO2	NO3	N2O5	OH
0.00	7.90000E+00 4.94404E-06	1.40000E+00	1.99000E+01	1.40000E+00	4.11000E-02	4.00000E+00	5.62874E-08	5.43045E-08	4.90202E-04
115.00	5.00000E+00 6.34440E-06	1.30000E+00	1.11000E+01	1.30000E+00	5.28000E-02	4.00000E+00	7.22580E-08	5.67402E-08	7.14142E-04
230.00	2.20000E+00 1.26180E-05	8.50000E-01	5.00000E+00	8.50000E-01	7.45000E-02	4.00000E+00	1.07378E-07	5.51302E-08	1.48804E-04
345.00	2.10000E+00 1.30890E-05	8.40000E-01	4.80000E+00	8.40000E-01	8.12000E-02	4.00000E+00	1.11148E-07	5.64045E-08	1.43104E-04
460.00	2.10000E+00 1.30890E-05	8.40000E-01	4.80000E+00	8.40000E-01	8.12000E-02	4.00000E+00	1.11148E-07	5.64045E-08	1.43104E-04

Figure 3.2a. DIFKIN Output of Initial Concentrations

DIFKIN SAMPLE SUB -

CP TIME = 37.00 DATE 02/25/79 PAGE 7

AN-38806 CONT.

CONCENTRATION PROFILES-PARTS PER HUNDRED MILLION

TIME = 3.00000E+01 MINUTES

GROUND DIFFUSIVITY = 30.000000

K1 = 4.7443200E-02

NITRIC OXIDE FLUX = 10.74800

HC FLUX = 33.673300

CO FLUX = 0.

WEIGHT-%	NO	NO2	HC	NO2	O2ON	HCN2	NO3	N2O5	OH
0.00	1.9184E+01 2.45712E-06	2.91308E+01	2.64382E+00	5.02100E-02	4.01010E+00	6.87110E-08	1.09727E-07	4.02874E-06	
115.00	4.43837E+00 1.12516E-05	1.14428E+01	2.26265E+00	1.41537E-01	3.99035E+00	2.48784E-07	3.39466E-07	1.08880E-05	
230.00	1.43403E+00 2.59335E-05	5.25554E+00	1.58444E+00	3.25974E-01	3.08235E+00	4.44010E-07	4.26852E-07	2.01612E-05	
345.00	1.41428E+00 2.90461E-05	4.69490E+00	1.50325E+00	3.52024E-01	3.98147E+00	4.81452E-07	4.37742E-07	2.18859E-05	
460.00	1.40524E+00 2.91802E-05	4.67007E+00	1.49066E+00	3.53218E-01	3.98143E+00	4.83280E-07	4.37772E-07	2.19454E-05	

NUMBER OF TIME STEPS IN CYCLE NO. 1 IS 121 DIFFERENTIAL CP TIME = 10.430

Figure 3.2b. DIFKIN Output of Computed Concentrations

3.3 UTILITY OUTPUTS

Several convenient utility outputs may be produced on an optional basis. These are:

- A list of all the time steps used in the integration (Table 2.1, card 13). This is written on logical unit 9.
- A note of the number of integration steps taken during a print interval and the central processor time used (Table 2.1, card 14; Fig. 3.2b).
- A list of the species concentrations (Fig. 3.2b) after every integration step rather than at every print interval (Table 2.1, card 15).

In addition to these we use peripheral units such as disks to print certain messages which assist the user in ascertaining that the run is proceeding properly. These messages are:

- The update time and updated value of the fluxes, k_1 , and diffusivities. The last are written on logical unit number 11, and the other two on logical unit number 10.
- The occurrence of negative concentrations. This is written on logical unit 8.

By means of control cards the user can cause these various messages to output to the line printer after program execution is terminated or, if desired, suppress the output.

4 TECHNIQUES FOR USING DIFKIN

4.1 CHANGING THE CHEMICAL MODEL

DIFKIN provides the user with great flexibility in changing the chemical model. The remarks that follow are intended to assist the user in changing models efficiently.

Changing the chemical model requires that new stoichiometric matrices be input (see Sec. 2.3.5). In this regard, it is important to keep in mind the need to be consistent in ordering the species and the reactions. For example, suppose that the reaction $\text{NO} + \text{NO}_3 \rightarrow 2\text{NO}_2$ were to be added to the reaction set shown in Fig. 3.1c, and let this be reaction number 17. Note that no new species have been added to the system. The first step that must be taken consists of changing the number of reactions from 16 to 17 (card 21, Appendix B). Then the appropriate rate constant and reaction description are inserted after cards 60 and 75 in Appendix B. The next step is to modify the stoichiometric matrices. This requires that a card be inserted for each species describing the stoichiometry of the species in the new reaction. Thus for NO we have to insert a card after card 91 in Appendix B which has a 1 in Column 1 and a zero in Column 11, since NO is a reactant but not a product. For hydrocarbon we have to insert a card after card 107 in Appendix B, containing zeros since hydrocarbon appears neither as a reactant nor a product in this reaction. And so on for the remaining species.

The procedure for adding a species is described below by means of an example. For simplicity, we assume that no new reactions are added. Thus suppose that in the present chemical model it is desired to compute explicitly the concentration of PAN in reaction 6, $\text{RO}_2 + \text{NO}_2 \rightarrow \text{PAN}$ (card 65, Appendix B; Fig. 3.1c). This adds one new species but no extra reactions. Suppose further that PAN is assigned position number 6 on the list of species. The first step is to increase the number of species in the input deck from 9 to 10 (card 22, Appendix B and Table 2.1). We

shall also assume that PAN is not in steady state, hence NSTDY (card 23, Appendix B and Table 2.1) does not change. The name and molecular weight of PAN must then be inserted after card 30 of Appendix B, and the initial concentration must be input after card 39 of Appendix B. The next step is to describe the stoichiometry of PAN. This is done by inserting 16 cards (one for each reaction) with the stoichiometric coefficients of PAN after card 155 of Appendix B. In this example PAN is a product of reaction 6 and does not appear in any other reaction. Hence the stoichiometry of PAN consists of zeroes on all cards except for reaction 6 which has a zero in Column 1 and a one in Column 11. Finally, the subroutines mentioned in the next paragraph must be modified since a new species has been added and the position of NO_3 , N_2O_5 , OH , and RO_2 in the species vector has been altered.

In addition to the changes in the inputs mentioned above, certain subroutines must be modified or changed altogether when the chemistry is changed. These are: JACOB, NUBETA, NURATE, STATE, and UPRATE. These subroutines must also be modified if the order of the species or the order of the reactions is changed. The reader is referred to Appendix A for an explanation of the contents of these subroutines.

4.2 MULTIPLE RUNS

DIFKIN is designed to allow the user to stack several cases using different inputs. It is presupposed, however, that the chemical model does not change from case to case, except that the values of the rate constants may be changed at will.

To run multiple cases it is required that a card which has the word "MORE" punched in Columns 1-4 be inserted between data decks. The program continues to read cards until either the word "END" or "MORE" is detected. The former causes execution to terminate; the latter causes the program to recycle and begin reading data.

When making multiple runs it is not necessary to input more than once the schematic description of the reaction set (see Sec. 2.3.4) and the stoichiometric matrices (see Sec. 2.3.5), since the basic chemical model does not change. All the other cards in the input deck must be input, however. For example, to run multiple cases using the sample deck shown in Appendix B, the user must omit cards 60 through 219 in any subsequent data decks, and include everything else.

4.3 DATE AND TIME SUBROUTINES

The code utilizes system routines for obtaining the date and the machine clock time. These system routines are peculiar to the computer center where the code is to be run and thus will require special handling at each installation. We have provided dummy routines which call the system routines in order to avoid the need to modify the main program. These dummy routines are MDATE and SECOND and are described in Appendix A.

5 PROGRAM MODIFICATIONS

This section contains information needed by the user in case certain basic modifications need to be carried out. The modifications consist of increasing the capacity of the program to allow for more species, more reactions, and more mesh points.

It may be recalled that the current array dimensions of the program limit the number of species and the number of reactions to 20 and the number of mesh points to 10. Tables 5.1, 5.2, and 5.3 show the arrays whose dimensions must be modified if more capacity is needed for species, reactions, and mesh points, respectively.

Additional changes that must be made in the main program are:

1. Change the 20 in the DATA statement DATA NROW/20/ to the new maximum number of species.
2. Change the 20 in the DATA statement DATA MAXR/20/ to the new maximum number of reactions.
3. Change the 10 in the DATA statement DATA MAXMSH/10/ to the new maximum number of space mesh points.

TABLE 5.1
DIMENSION CHANGES REQUIRED TO ADD MORE SPECIES

Array	Location	Modification Instructions*
ISTOYR	COMMON/CHEM/	C = MNS
RATE	COMMON/CHEM/	R = MNS
BETA	COMMON/CHEM/	C = MNS
CONIN	COMMON/CHEM/	R = MNS
WTMOLE	COMMON/CHEM/	Length = MNS
II	COMMON/CHEM/	Length = MNS × MNR
JJ	COMMON/CHEM/	Length = MNS + 1
VALWAL	COMMON/TRACER/	Length = MNS
FLXWAL	COMMON/TRACER/	Length = MNS
FLXDGE	COMMON/TRACER/	Length = MNS
STOYKR	Main Program	C = MNS
STOYKP	Main Program	C = MNS
SPEC	Main Program	Length = MNS
CONUP	Main Program	R = MNS
CONEW	Main Program	R = MNS
PPHM	Main Program	R = MNS
WORK	Main Program	R = MNS
GZERO	Main Program	R = MNS
AJACOB	Main Program	R = MNS, C = MNS × MNP
Q	Main Program	R = MNS, C = MNS × MNP

*
 R = number of rows of a two-dimensional array
 C = number of columns of a two-dimensional array
 MNS = maximum number of species
 MNR = maximum number of reactions
 MNP = maximum number of mesh points

TABLE 5.2
DIMENSION CHANGES REQUIRED TO ADD MORE REACTIONS

Array	Location	Modification Instructions*
ISTOYR	COMMON/CHEM/	R = MNR
BETA	COMMON/CHEM/	R = MNR
RATEFF	COMMON/CHEM/	Length = MNR
RATKON	COMMON/CHEM/	Length = MNR
II	COMMON/CHEM/	Length = MNR × MNS
STOYKR	Main Program	R = MNR
STOYKP	Main Program	R = MNR
REACT	Main Program	R = MNR

*
 R = number of rows of a two-dimensional array
 C = number of columns of a two-dimensional array
 MNS = maximum number of species
 MNR = maximum number of reactions
 MNP = maximum number of mesh points

TABLE 5.3
DIMENSION CHANGES REQUIRED TO ADD MORE SPACE MESH POINTS

Array	Location	Modification Instructions *
RATE	COMMON/CHEM/	C = MNP
CONIN	COMMON/CHEM/	C = MNP
DFINIT	COMMON/SKY/	Length = MNP + 1
ZEE	COMMON/SKY/	Length = MNP
TRACIN	COMMON/TRACER/	Length = MNP
SCALDF	COMMON/TRACER/	Length = MNP + 1
CONUP	Main Program	C = MNP
CONEW	Main Program	C = MNP
PPHM	Main Program	C = MNP
WORK	Main Program	C = MNP
GZERO	Main Program	C = MNP
AJACOB	Main Program	C = MNP × MNS
Q	Main Program	C = MNP × MNS
SCALE	Main Program	Length = MNP
DSCALE	Main Program	Length = MNP
DCOF	Main Program	Length = MNP
HTINV	Main Program	C = MNP + 3
TRIDAT	Subroutine CRANK	Length = (4 × MNP) - 2

*
R = number of rows of a two-dimensional array
C = number of columns of a two-dimensional array
MNS = maximum number of species
MNR = maximum number of reactions
MNP = maximum number of mesh points

6 CONTROL OF INTEGRATION STEP SIZE

The parameters TSTMAX and TSTMIN control the size of the integration step (see Table 2.1, cards 5 and 6). The step size is controlled by a fractional-change criterion as follows. Let the concentration of the i th species at the j th mesh point at the n th step be denoted by c_{ij}^n . The test performed uses the fractional change parameter

$$\alpha_{ij} = |c_{ij}^{n+1} - c_{ij}^n| / c_{ij}^n$$

If $\alpha_{ij} > \text{TSTMAX}$ for any (i,j) combination, the step size is halved for the next integration cycle. If $\alpha_{ij} < \text{TSTMIN}$ for all i and j , the step size is doubled for the next integration cycle. For any particular problem some experimentation is required to determine the values of TSTMAX and TSTMIN that yield a good combination of speed and accuracy. Our experience has been that values of $\text{TSTMAX} = .03$ and $\text{TSTMIN} = .01$ work very well for the current model.

APPENDIX A

LIST OF SUBROUTINES AND THEIR USE

A.1 SUBROUTINE COEQ(N,A,X,FL)

Use. Solves a set of simultaneous linear equations whose matrix is tridiagonal. In DIFKIN it is used to solve the equations which yield the concentration of the tracer species. It is called by subroutine CRANK.

Arguments. N = number of rows in the matrix
 A = matrix elements stored in a linear vector of
 4N - 2 elements
 X = solution vector
 FL = failure index: FL = 1 if matrix is singular, and
 FL = 0 otherwise

Remarks. The nonzero elements of the vector A look like

Row 1	A(1)	A(2)			A(3)
2	A(4)	A(5)	A(6)		A(7)
3		A(8)	A(9)	A(10)	A(11)
.....					...
N-2			A(4N-12)	A(4N-11)	A(4N-10) A(4N-9)
N-1				A(4N-8)	A(4N-7) A(4N-6) A(4N-5)
Row N					A(4N-4) A(4N-3) A(4N-2)

A.2 SUBROUTINE CRANK(N,DELT)

Use. Solves the linear diffusion equation $\partial c / \partial t = \partial / \partial z [D(z) \partial c / \partial z]$, which has a diffusion coefficient which is a function of z. Uses the Crank-Nicolson method of differencing. Used with inert species only.

Arguments. N = number of mesh points
 DELT = integration step size

Remarks. Calls subroutine COEQ for solving the resulting system of equations. The concentrations and other variables are passed through COMMON/TRACER/.

A.3 SUBROUTINE DFFUSE(NOSTAT, DELZ)

Use. Sets initial values of diffusion coefficients when diffusivities are not time-varying. The diffusivities are stored in the vector DFINIT, which is transferred to the subroutine through COMMON/SKY/.

Arguments. NOSTAT = number of mesh points
DELZ = mesh interval

A.4 SUBROUTINE DIFCOF(SCALDF, NOSTAT, DCOF, SCALE, DSCALE)

Use. Generates scaling vectors DCOF, SCALE, DSCALE, for use in the integration of the rate equations of the reactive species.

Arguments. SCALDF = input vector of scaled diffusivities, defined in main program by $SCALDF(I) = D(I)/DELZ^2$, where $D(I)$ = ith diffusivity and DELZ = mesh interval.

NOSTAT = number of mesh points

DCOF = a vector used for scaling the matrix equation which is the result of the finite-difference method. $DCOF(I) = SCALDF(I) + SCALDF(I+1)$

SCALE = vector of scale factors

$SCALE(I) = SCALDF(I+1)/SCALDF(I)$

DSCALE = vector of scale factors

$DSCALE(I) = 1/SCALDF(I)$

A.5 SUBROUTINE JACOB(A,B,R,N,W,NN,C)

Use. Computes the Jacobian matrix of the chemical rate equations having the form $dy_i/dt = f_i(y_1, y_2, \dots, y_n)$, where y_i is the concentration of the i th species, $i = 1, 2, \dots, N$. Each element of the Jacobian is defined by $A_{ij} = \partial f_i / \partial y_j$, $i, j = 1, 2, \dots, N$.

Arguments. A = Jacobian matrix of size $N \times N$
B = vector of species concentrations
R = vector of chemical rate constants
N = order of the Jacobian matrix, equal to the number of rate equations to be integrated
W = vector of molecular weights of all the chemical species
NN = total number of species in the system, including species in steady-state but not the tracer species
C = work vector

A.6 SUBROUTINE MATADD(A,B,C,NRA,NCA)

ENTRY MATSUB(A,B,C,NRA,NCA)

Use. MATADD computes the sum of two matrices $C = A + B$
MATSUB computes the difference of two matrices $C = A - B$

Arguments. A, B = input matrices
C = resultant matrix
NRA = number of rows of A, B, C
NCA = number of columns of A, B, C

A.7 SUBROUTINE MATINV(A,N,NMAX,B,M,PIVOT,IPIVOT,INDEX,DETERM)

Use. Computes the inverse of the matrix A or the solution of the matrix equation $Ax = B$. Called by MATNVT.

Arguments.

A = matrix to be inverted of order $N \times N$

N = order of matrix A

NMAX = dimension of A as declared in calling program,
 $NMAX \geq N$

B = right-hand side of matrix equation $Ax = B$,
dimensioned B(NMAX,M)

M = number of columns of B; if $M \leq 0$ only the
matrix inverse is found, without solving
matrix equations

PIVOT = work vector of size N

IPIVOT = work vector of size N

INDEX = work array dimensioned INDEX(N,2)

DETERM = determinant of A

A.8 SUBROUTINE MATMUL(A,B,C,NRA,NCARB,NCB)

Use. Computes the matrix product $C = A \times B$.

Arguments.

A = matrix of order $NRA \times NCARB$

B = matrix of order $NCARB \times NCB$

$C = A \times B$

NRA = number of rows of A

NCARB = number of columns of A and rows of B

NCB = number of columns of B

A.9 SUBROUTINE MATNVT(A,N,D)

Use. Computes the inverse of matrix A by calling MATINV.

Arguments. A = matrix of order $N \times N$; destroyed in the inversion
process as its inverse is substituted for it

N = order of matrix A, limited to 24

D = determinant of A

A.10 SUBROUTINE MATSCL(X,A,NR,NC)

Use. Scales the matrix A by factor X.

Arguments. X = scaling factor

A = matrix to be scaled

NR = number of rows of A

NC = number of columns of A

A.11 SUBROUTINE MDATE(IDATE)

Use. This is a dummy subroutine which calls other system routines to obtain the date of the run. The date is printed on every page of the output. User must modify MDATE in order to make it compatible with his installation.

Argument. IDATE = vector which contains the date of the run

A.12 SUBROUTINE NEWPAG(TITLE,LSKIP,IDATE)

Use. This is a utility subroutine used for labeling each page of the output. The subroutine labels each page with the run label provided by the user, the date of the run, the internal machine time, and the page number.

Arguments. TITLE = vector of Hollerith characters which contains the run label which user prescribed in the first card of the input deck (see Table 2.1, card 1)

LSKIP = number of lines skipped before printing heading;
if LSKIP = 0 the page heading is printed at the top of the page

IDATE = vector which contains the date of the run

A.13 SUBROUTINE NUBETA(BETA,NR)

Use. Used to modify the net stoichiometric matrix when required by stationarity assumptions.

Arguments. BETA = net stoichiometric matrix;

$$\text{BETA}(i,j) = v'_{ij} - v_{ij}, \quad i = 1, 2, \dots, r, \quad j = 1, 2, \dots, s,$$

where r = number of reactions and s = number of species (see Sec. 2.3.5 for definition of v'_{ij} and v_{ij})

NR = number of rows of BETA as declared in DIMENSION statement

A.14 SUBROUTINE NURATE(RATEFF,RATKON,CONUP)

Use. This routine computes any pseudo-rate constants which result from stationarity assumptions.

Arguments. RATEFF = vector of effective rate constants which contains all the pseudo-rate constants

RATKON = vector of basic rate constants which are used to compute the pseudo-rate constants

CONUP = vector of species concentrations

A.15 SUBROUTINE PREDAT

Use. Reads input data from card reader and produces a listing of the image of the input deck. See Sec. 2.1 for a full explanation.

A.16 SUBROUTINE QGEN(A,B,C,N)

Use. This subroutine generates the Q matrix which enters into the matrix equation $Q(C - C_0) = -2G_0$. The Q matrix is stored in the same location as the matrix A and is defined by

$$Q_{ij} = -C \times A_{ij}, \quad Q_{jj} = B - A_{jj}$$

Arguments. A = matrix of order $N \times N$, modified by the subroutine
 B = constant factor added to the diagonal elements of A
 C = constant factor which scales all the elements of A
 N = order of matrix A

A.17 SUBROUTINE SECOND(A)

Use. This is a dummy subroutine which calls other system routines to obtain the internal machine time. It is used by the main program for timing the computation. It is also called by NEWPAG.

Arguments. A = internal machine time in any desired units

A.18 SUBROUTINE SOURCE(CONUP)

Use. Computes the rate function of the chemical rate equations.

Arguments. CONUP = work vector

Remarks. Consider a set of chemical equations defined by:

$$\sum_{j=1}^s v_{ij} M_j \xrightarrow{k_i} \sum_{j=1}^s v'_{ij} M_j \quad i = 1, 2, \dots, r$$

where M_j = chemical formula of the j th species
 k_i = rate constant of i th reaction
 v_{ij} = stoichiometric coefficient of j th reactant in the i th reaction
 v'_{ij} = stoichiometric coefficient of the j th product in the i th reaction
 r = number of reactions
 s = number of species

The rate equations for such a system are defined by:

$$\frac{dc_j}{dt} = R_j = \sum_{i=1}^r (v'_{ij} - v_{ij}) k_i \prod_{m=1}^s c_m^{v_{im}} \quad ; \quad j = 1, 2, \dots, s$$

where c_j = concentration of the j th species

R_j = rate function of the j th species

Subroutine SOURCE computes R_j as shown above. The quantities needed by SOURCE are provided through COMMON/CHEM/.

A.19 SUBROUTINE STATE(CONEW,CONUP,NROW)

Use. Computes algebraically the concentrations of those species assumed to be in steady state.

Arguments. CONEW = array of updated species concentrations; CONEW(i,j) is the concentration of the i th species at the j th mesh point

CONUP = work vector

NROW = number of rows of CONEW as declared in a DIMENSION statement

Remarks. Other quantities needed by STATE are provided through COMMON/CHEM/. This subroutine must be modified when the chemical model is changed or the order of the species and reactions is altered.

A.20 SUBROUTINE TIMEX(KSTEP,TITLE,IDATE)

Use. This subroutine is used for timing various phases of the computational process. It also counts the number of integration steps during a print interval.

Arguments. KSTEP = total number of integration steps taken to date

TITLE = Hollerith vector which contains the label of output page

IDATE = vector which contains the date of the run

Remarks. This subroutine contains an entry called ENDRUN which is called at the end of the computation to compute and print the net time

taken by the computation. Subroutine TIMEX calls subroutines SECOND and NEWPAG.

A.21 SUBROUTINE TRIVRT(A,D,SCALE,WORK,NRA,NCA,NMAT,NNR,U)

Use. Inverts a tridiagonal matrix, A, whose elements also are matrices. The lower-diagonal entries are identity matrices. The upper-diagonal elements are scaled identity matrices.

Arguments.

A = doubly-dimensioned array of size NRA × NCA

D = array of size NRA × NMAT; right-hand side of matrix equation

SCALE = vector of scale factors of the upper-diagonal elements of A

WORK = work array of size NRA × NRA

NRA = number of rows of A as declared in a DIMENSION statement in the calling program

NCA = number of columns of A, NCA = NRA × NMAT

NMAT = number of columns of D

NNR = actual order of the diagonal elements of A

U = solution array of size NRA × NMAT

Remarks. Given a matrix equation of the form

$$AU = D$$

where A is block tridiagonal, this subroutine computes the solution U.

The form of A is

$$A = \begin{bmatrix} A_{11} & \alpha_1 I & 0 & \dots & 0 \\ I & A_{22} & \alpha_2 I & \dots & 0 \\ \dots & \dots & \dots & \dots & \dots \\ 0 & & I & A_{N-1,N-1} & \alpha_{N-1} I \\ 0 & & 0 & I & A_{NN} \end{bmatrix}$$

where $N = \text{NMAT}$, and the α_i 's correspond to the scale factors stored in SCALE. It can be seen that there is no need to store A in full since only the diagonal elements, A_{ii} , are important. The zeros can be excluded, of course, and the identity matrices are known and need not be stored. Thus the matrix A that is input into TRIVRT contains only the diagonal elements, A_{ii} , of the full matrix. Each A_{ii} is of order NNR, and the first entry of each A_{ii} is stored in A_{ij} , where $j = (i-1)\text{NRA} + 1$, $i = 1, \dots, \text{NMAT}$. Thus the actual A looks like

$$A = \underbrace{[A_{11}, A_{22}, \dots, A_{N-1, N-1}, A_{NN}]}_{\text{NMAT} \times \text{NRA}} \} \text{NRA}$$

Similarly, U and D are stored in the form

$$U = \underbrace{[U_1, U_2, \dots, U_N]}_{\text{NMAT}} \} \text{NRA}$$

$$D = \underbrace{[D_1, D_2, \dots, D_N]}_{\text{NMAT}} \} \text{NRA}$$

and each U_i and D_i is a vector of NRA components..

A.22 SUBROUTINE UPFLUX(TIME,NTRACE)

Use. This subroutine is called by the main program at time TIME to update the fluxes.

Arguments. TIME = time at which fluxes are updated

NTRACE = flag which tells the subroutine whether or not a tracer species is present (see Table 2.1, card 24)

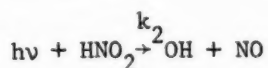
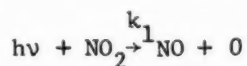
Remarks. The fluxes are scaled by a factor of 10^8 for the purpose of improving computational accuracy in the integration process. Any required additional scaling of the fluxes must be done by this subroutine. The subroutine prints a message on logical unit 10 which lets the user know the update time and the value of the new fluxes.

A.23 SUBROUTINE UPRATE(TIME,RATNEW,RATOLD,RATEFF)

Use. This subroutine is used to update the magnitude of rate constants which are functions of time.

Arguments. TIME = update time
 RATNEW = factor used for updating the rate constant
 RATOLD = vector of old rate constants to be updated
 RATEFF = work vector of old rate constants

Remarks. In our photochemical smog model there are two reactions which are directly triggered by sunlight. They are:



As sunlight intensity changes with time of day both k_1 and k_2 must be updated. In our model k_2 is a function of k_1 and thus the variable RATNEW is actually the new value of k_1 . Then k_2 is computed from k_1 and stored in the appropriate location in both RATOLD and RATEFF. The new value of k_1 is also stored in these two vectors.

A.24 SUBROUTINE WXMIT(NWDS,NCLS,SF,FROM,TO)

Use. This subroutine is used to transfer scaled values of array FROM to vector TO.

Arguments. NWDS = number of words to be transferred; if NWDS < 0,
then the quantity SF × FROM(1,1) is transferred
to NWDS locations in TO.

NCLS = number of rows of FROM

SF = scale factor

FROM = two-dimensional array

TO = vector that receives scaled elements of FROM

A.25 SUBROUTINE XMIT(N,A,B)

Use. Transmits N words from A to B.

Arguments. N = number of words to be transmitted; if N < 0,
subroutine transmits A to N locations in B

A = value of vector to be transmitted

B = vector receiving new values

APPENDIX B

LISTING OF INPUT DECK PRODUCED BY SUBROUTINE PREDAT

THAMES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
1	*****							
1	DIFKIN SAMPLE RUN -							
2	INITIAL TIME				0.			
3	FINAL TIME				360.			
4	INITIAL TIME STEP				.01			
5	UPPER LIMIT FRACTIONAL CHANGE				.03			
6	LOWER LIMIT FRACTIONAL CHANGE				0.01			
7	PRINT INTERVAL				30.			
8	UPPER LIMIT ON DELT				0.5			
9	LOWER LIMIT ON DELT				0.002			
10	VERTICAL MESH INTERVAL (METERS)				115.			

CARD	1	11	21	31	41	51	61	71
11	*****							
11	TIME INTERVAL FOR UPDATING K1				10.			
12	DO WE WANT A FIXED STEP SIZE				NO			
13	SHALL WE OUTPUT THE TIME STEPS				NO			
14	SHALL WE OUTPUT THE EXECUTION TIMES				YES			
15	SHALL WE OUTPUT EVERY CYCLE				NO			
16	DO WE WANT PUNCHED OUTPUT				NO			
17	IS K1 VARIABLE				YES			
18	ARE SOURCES TIME-VARIABLE				YES			
19	IS INVERSION HEIGHT VARIABLE				YES			
20	NUMBER OF INTEGRATION STEPS				25000			

CARD	1	11	21	31	41	51	61	71
21	*****							
21	NUMBER OF REACTIONS				16			
22	NUMBER OF SPECIES				9			
23	NUMBER OF SPECIES IN STEADY STATE				4			
24	NUMBER OF TRACER SPECIES (0 OR 1)				0			
25	NUMBER OF VERTICAL STATIONS				5			
26	SPECIES NAME AND MOLE WEIGHT				NO 30.01			
27					HC 72.20			
28					NO2 46.01			
29					OZON 48.			
30					HNO2 47.00			

CARD	1	11	21	31	41	51	61	71
31	*****							
31					NO3 62.			
32					N2O5 108.			
33					OH 17.			
34					PO2 68.1			
35	NO PPHM 7.9 5.0				2.2 2.1			
36	HC PPHM 19.9 11.1				5.0 4.8 4.8			
37	NO2 PPHM 1.6 1.3				0.85 0.84 0.84			
38	O3 PPHM .0411 .0528				.0785 .0812 .0812			
39	HNO2 PPHM 4. 4.				4. 4. 4.			
40	NO3 PPHM = COMPUTED							

BY CODE

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
41	N2O5 PPHN= COMPUTED							
42	OH PPHN= COMPUTED							
43	RO2 PPHN= COMPUTED							
44	RATE CONSTANTS -							
45	REACTION NO. 1 (K1)							
46	REACTION NO. 2 .267							
47	REACTION NO. 3 1.000E-6							
48	REACTION NO. 4 50.							
49	REACTION NO. 5 1.0E+3							
50	REACTION NO. 6 2.0							
	REACTION NO. 7 15.							

BY CODE
BY CODE
BY CODE

OBTAINED FROM -UPRATE-

CARD	1	11	21	31	41	51	61	71
51	REACTION NO. 8 30.							
52	REACTION NO. 9 4.00E-5							
53	REACTION NO. 10							
54	REACTION NO. 11 5.0E-5							
55	REACTION NO. 12 45.							
56	REACTION NO. 13 14.							
57	REACTION NO. 14 60.5							
58	REACTION NO. 15 1.0E-5							
59	REACTION NO. 16 .001							
60	PHOTON + NO2 = NO + O3							

OBTAINED FROM -UPRATE-

CARD	1	11	21	31	41	51	61	71
61	NO + O3 = NO2 + O2							
62	O + HC = BR02							
63	OH + HC = BR02							
64	RO2 + NO = NO2 + .125*OH							
65	RO2 + NO2 = PAN							
66	OH + NO = HN02							
67	OH + NO2 = HN03							
68	O3 + HC = RO2							
69	PHOTON + HN02 = OH + NO							
70	NO2 + O3 = NO3 + O2							

CARD	1	11	21	31	41	51	61	71
71	NO3 + NO2 = N2O5							
72	N2O5 = NO3 + NO2							
73	N2O5 + H2O = 2HN03							
74	NO + NO2 + H2O = 2HN02							
75	NO2 + PARTICLES = PRODUCTS							
76	0.	1.	BEGIN NO					
77	1.	0	STOICHIOMETRIC COEFFICIENTS					
78	0	0						
79	0	0						
80	1.	0						

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
81	0	0						
82	1.	0						
83	0	0						
84	0	0						
85	0	1.						
86	0.	0.						
87	0.	0.						
88	0.	0.						
89	0.	0.						
90	1.	0.						

CARD	1	11	21	31	41	51	61	71
91	0.	0.						
92	0.	0.						
93	0	0						
94	1.	0.						
95	1.	0						
96	0	0						
97	0	0						
98	0	0						
99	0	0						
100	1.	0						

END NO
BEGIN HYDROCARBON

CARD	1	11	21	31	41	51	61	71
101	0	0						
102	0	0						
103	0.	0.						
104	0.	0.						
105	0.	0.						
106	0.	0.						
107	0.	0.						
108	1.	0.						
109	0	1.						
110	0	0						

END HYDROCARBON
BEGIN NO2

CARD	1	11	21	31	41	51	61	71
111	0	0						
112	0	1.						
113	1.	0						
114	0	0						
115	1.	0						
116	0	0						
117	0	0						
118	1.	0						
119	1.	0.						
120	0.	1.						

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
121	0	0						
122	1.	0.						
123	1.	0.						
124	0.	1.						
125	1.	0						
126	0	0						
127	0	0						
128	0	0						
129	0	0						
130	0	0						

END N02
BEGIN OZONE

CARD	1	11	21	31	41	51	61	71
131	0							
132	1.	0						
133	0	0						
134	1.	0.						
135	0.	0.						
136	0.	0.						
137	0.	0.						
138	0.	0.						
139	0.	0.						
140	0.	0.						

END OZONE
BEGIN HN02

CARD	1	11	21	31	41	51	61	71
141	0	0						
142	0	0						
143	0	0						
144	0	0						
145	0	0						
146	0	1.						
147	0	0						
148	0	0						
149	1.	0						
150	0	0						

CARD	1	11	21	31	41	51	61	71
151	0.	0.						
152	0.	0.						
153	0.	0.						
154	0.	2.						
155	0.	0.						
156	0.	0.						
157	0	0						
158	0	0						
159	0	0						
160	0	0						

END HN02
BEGIN N03

IMAGES OF DATA-CARDS

	1	11	21	31	41	51	61	71
CARD	0.	0.						
161	0.	0.						
162	0.	0.						
163	0.	0.						
164	0.	0.						
165	0.	0.						
166	0.	1.						
167	1.	0.						
168	0.	1.						
169	0.	0.						
170	0.	0.						

	1	11	21	31	41	51	61	71
CARD	0.	0.						
171	0.	0.						
172	0.	0.						
173	0.	0.						
174	0.	0.						
175	0.	0.						
176	0.	0.						
177	0.	0.						
178	0.	0.						
179	0.	0.						
180	0.	0.						

END N03
BEGIN N205

	1	11	21	31	41	51	61	71
CARD	0.	0.						
181	0.	0.						
182	0.	0.						
183	0.	1.						
184	1.	0.						
185	1.	0.						
186	0.	0.						
187	0.	0.						
188	0.	0.						
189	0.	0.						
190	0.	0.						

END N205
BEGIN OM

	1	11	21	31	41	51	61	71
CARD	0.	0.						
191	1.	0.						
192	0.	0.125						
193	0.	0.						
194	1.	0.						
195	1.	0.						
196	0.	0.						
197	0.	1.						
198	0.	0.						
199	0.	0.						
200	0.	0.						

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
201	0.	0.						
202	0.	0.						
203	0.	0.						
204	0.	0.						
205	0	0						
206	0.	8.						
207	0.	8.						
208	1.	0						
209	1.	0						
210	0	0						

END ON
BEAM R02

CARD	1	11	21	31	41	51	61	71
211	0	0						
212	0.	1.						
213	0	0						
214	0	0						
215	0.	0.						
216	0.	0.						
217	0.	0.						
218	0.	0.						
219	0.	0.						
220	630	K1						

END R02
5.42339E-02

END STOICHIOMETRY

CARD	1	11	21	31	41	51	61	71
221	640			7.62301E-02				
222	650			9.74432E-02				
223	700			1.17867E-01				
224	710			1.37498E-01				
225	720			1.56330E-01				
226	730			1.74362E-01				
227	740			1.91591E-01				
228	750			2.08016E-01				
229	800			2.23639E-01				
230	810			2.38459E-01				

CARD	1	11	21	31	41	51	61	71
231	820			2.52479E-01				
232	830			2.65703E-01				
233	840			2.78136E-01				
234	850			2.89783E-01				
235	900			3.00651E-01				
236	910			3.10749E-01				
237	920			3.19340E-01				
238	930			3.27962E-01				
239	940			3.35882E-01				
240	950			3.43111E-01				

IMAGES OF DATA-CARDS

	1	11	21	31	41	51	61	71
CARD	1	11	21	31	41	51	61	71
241	1000			3.49661E-01				
242	1010			3.55543E-01				
243	1020			3.60771E-01				
244	1030			3.65358E-01				
245	1040			3.69320E-01				
246	1050			3.72670E-01				
247	1100			3.75422E-01				
248	1110			3.77590E-01				
249	1120			3.79183E-01				
250	1130			3.80211E-01				

	1	11	21	31	41	51	61	71
CARD	1	11	21	31	41	51	61	71
251	1140			3.80679E-01				
252	1150			3.80591E-01				
253	1200			3.79946E-01				
254	1210			3.78740E-01				
255	1220			3.76966E-01				
256	1230			3.74614E-01				
257	1240			3.71674E-01				
258	1250			3.68131E-01				
259	1300			3.63971E-01				
260	1310			3.59181E-01				

	1	11	21	31	41	51	61	71
CARD	1	11	21	31	41	51	61	71
261	1320			3.53746E-01				
262	1330			3.47653E-01				
263	1340			3.40887E-01				
264	1350			3.33437E-01				
265	1400			3.25292E-01				
266	1410			3.17193E-01				
267	1420			3.07610E-01				
268	1430			2.97263E-01				
269	1440			2.86143E-01				
270	1450			2.74240E-01				

	1	11	21	31	41	51	61	71
CARD	1	11	21	31	41	51	61	71
271	1500			2.61549E-01				
272	1510			2.48064E-01				
273	1520			2.33780E-01				
274	1530			2.18694E-01				
275	1540			2.02803E-01				
276	1550			1.86108E-01				
277	1600			1.68608E-01				
278	1610			1.50304E-01				
279	1620			1.31198E-01				
280	1630			1.11293E-01				

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
201	1640			9.05928E-02				
202	1650			4.91033E-02				
203	1700			4.68362E-02				
204	LAST CARD K1			-10.				
205	DIFF. UPDATE		0.	0.	30.	30.	30.	
206			30.	30.	30.			
207	DIFF. UPDATE		150.	57.5	30.	600.	30.	
208			30.	30.	30.			
209	DIFF. UPDATE		225.	172.5	60.	600.	600.	
290			30.	30.	30.			

CARD	1	11	21	31	41	51	61	71
291	DIFF. UPDATE		300.	287.5	600.	600.	600.	
292			600.	30.	30.			
293	DIFF. UPDATE		375.	402.5	600.	600.	600.	
294			600.	600.	30.			
295	DIFF. UPDATE		390.	460.	600.	600.	600.	
296			600.	600.	600.			
297	LAST CARD		-10.					
298	2ND LAST CARD							
299	FLUX TIMES		430		0.	TIME MATCHES INITIAL RUN TIME		
300			635		5.			

CARD	1	11	21	31	41	51	61	71
301			640		10.			
302			641		11.			
303			650		20.			
304			653		23.			
305			700		30.			
306			705		35.			
307			710		40.			
308			715		45.			
309			718		48.			
310			720		50.			

CARD	1	11	21	31	41	51	61	71
311			751		81.			
312			752		82.			
313			800		90.			
314			820		110.			
315			839		129.			
316			840		130.			
317			855		145.			
318			860		150.			
319			900		150.			
320			900		150.			

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
321			910					
322			920					
323			921					
324			939					
325			1000					
326			1003					
327			1026					
328			1043					
329			1100					
330			1112					

CARD	1	11	21	31	41	51	61	71
331			1113					
332			1130					
333			1143					
334			1200					
335			1202					
336			1212					
337			1230					
338	LAST CARD OF VECTOR OF FLUX TIMES				-10.	TIME MATCHES FINAL RUN TIME		
339	NO		630	FLUXES	3.07086E-07	HAS DUMMY NEGATIVE FLUX TIME		
340	MC		630		5.44323E-07			

CARD	1	11	21	31	41	51	61	71
341	NO		635		3.07086E-07			
342	MC		635		5.46873E-07			
343	NO		640		3.07086E-07			
344	MC		640		5.49782E-07			
345	NO		641		3.41468E-07			
346	MC		641		6.44693E-07			
347	NO		650		3.41468E-07			
348	MC		650		6.51445E-07			
349	NO		653		1.07495E-07			
350	MC		653		3.36733E-07			

CARD	1	11	21	31	41	51	61	71
351	NO		700		1.72669E-07			
352	MC		700		4.54057E-07			
353	NO		705		1.72669E-07			
354	MC		705		4.53212E-07			
355	NO		710		1.72669E-07			
356	MC		710		4.52155E-07			
357	NO		715		1.72669E-07			
358	MC		715		4.51309E-07			
359	NO		718		2.01891E-07			
360	MC		718		5.03024E-07			

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
361	NO		720		2.01891E-07			
362	MC		720		5.02795E-07			
363	NO		751		1.72669E-07			
364	MC		751		4.50665E-07			
365	NO		752		4.82533E-07			
366	MC		752		8.75117E-07			
367	NO		800		4.35924E-07			
368	MC		800		8.16496E-07			
369	NO		820		4.35924E-07			
370	MC		820		8.09878E-07			

CARD	1	11	21	31	41	51	61	71
371	NO		839		3.92953E-07			
372	MC		839		6.80554E-07			
373	NO		840		3.92953E-07			
374	MC		840		6.80012E-07			
375	NO		855		3.92953E-07			
376	MC		855		6.73708E-07			
377	NO		860		1.37077E-07			
378	MC		860		3.11906E-07			
379	NO		900		1.12553E-07			
380	MC		900		2.61723E-07			

CARD	1	11	21	31	41	51	61	71
381	NO		900		1.60145E-07			
382	MC		900		2.76219E-07			
383	NO		910		1.60145E-07			
384	MC		910		2.76796E-07			
385	NO		920		1.60145E-07			
386	MC		920		2.76994E-07			
387	NO		921		7.69501E-08			
388	MC		921		1.66346E-07			
389	NO		939		1.92561E-07			
390	MC		939		3.37212E-07			

CARD	1	11	21	31	41	51	61	71
391	NO		1000		1.84549E-07			
392	MC		1000		3.27966E-07			
393	NO		1003		9.66976E-08			
394	MC		1003		2.08196E-07			
395	NO		1026		1.07797E-07			
396	MC		1026		2.40371E-07			
397	NO		1043		1.75130E-07			
398	MC		1043		2.54872E-07			
399	NO		1100		1.96305E-07			
400	MC		1100		2.90872E-07			

IMAGES OF DATA-CARDS

CARD	1	11	21	31	41	51	61	71
401	NO		1112		1.05725E-07			
402	MC		1112		2.32002E-07			
403	NO		1113		7.84901E-08			
404	MC		1113		1.88121E-07			
405	NO		1130		7.84901E-08			
406	MC		1130		1.88576E-07			
407	NO		1143		9.39590E-09			
408	MC		1143		2.67180E-08			
409	NO		1200		9.39590E-09			
410	MC		1200		2.67180E-08			

CARD	1	11	21	31	41	51	61	71
411	NO		1202		3.34155E-08			
412	MC		1202		1.05322E-07			
413	NO		1212		6.11234E-08			
414	MC		1212		1.52622E-07			
415	NO		1230		6.11234E-08			
416	MC		1230	END FLUX	1.52622E-07			
417	END	NOTE TO USER- FOR STACKING RUNS WRITE MORE INSTEAD OF END IN COLS. 1-4						

APPENDIX C
COMMON BLOCKS

Three COMMON blocks are used in DIFKIN. The locations of these blocks are shown in Table C.1. All three blocks are located in the main program also.

TABLE C.1
SUBROUTINE LOCATION OF COMMON BLOCKS*

COMMON Block Name	Subroutine Location
CHEM	SOURCE, STATE
SKY	DFFUSE
TRACER	CRANK, UPFLUX

* All COMMON blocks are also found in the main program.

REFERENCES

1. A. Q. Eschenroeder and J. R. Martinez, Further Development of the Photochemical Smog Model for the Los Angeles Basin, General Research Corporation CR-1-191, March 1971.

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